

=> fil reg

FILE 'REGISTRY' ENTERED AT 08:32:31 ON 05 SEP 2000
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STRUCTURE FILE UPDATES: 4 SEP 2000 HIGHEST RN 288141-13-9
DICTIONARY FILE UPDATES: 4 SEP 2000 HIGHEST RN 288141-13-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

Please note that search-term pricing does apply when
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Structure search limits have been increased. See HELP SLIMIT
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=> d sta que 120

L20 1 SEA FILE=REGISTRY ABB=ON PLU=ON (LMYPTYLK)/SQEP

=> d his 120-122

(FILE 'REGISTRY' ENTERED AT 08:24:03 ON 05 SEP 2000)

L20 1 S E3
E 'LEU-MET-TYR-PRO-THR-TYR-LEU-LYS'/SQEP
E 'AIB-MET-TYR-PRO-THR-TYR-AIB-LYS'/SQEP
E 'LEU-MET-TYR-PRO-THR-TYR-AIB-LYS'/SQEP
E 'AIB-MET-TYR-PRO-THR-TYR'/SQEP
E 'LEU-MET-TYR-PRO-THR-TYR'/SQEP

FILE 'HCAOLD' ENTERED AT 08:30:44 ON 05 SEP 2000

L21 0 S L20

FILE 'HCAPLUS' ENTERED AT 08:30:49 ON 05 SEP 2000

L22 4 S L20

=> d 120 sqide can

L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2000 ACS

RN 120550-85-8 REGISTRY

CN L-Lysine, N2-[N-[N-[N-[1-[N-(N-L-leucyl-L-methionyl)-L-tyrosyl]-L-prolyl]-L-threonyl]-L-tyrosyl]-L-leucyl]- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 8

SEQ 1 LMYPTYLK

=====

HITS AT: 1-8

MF C50 H77 N9 O12 S

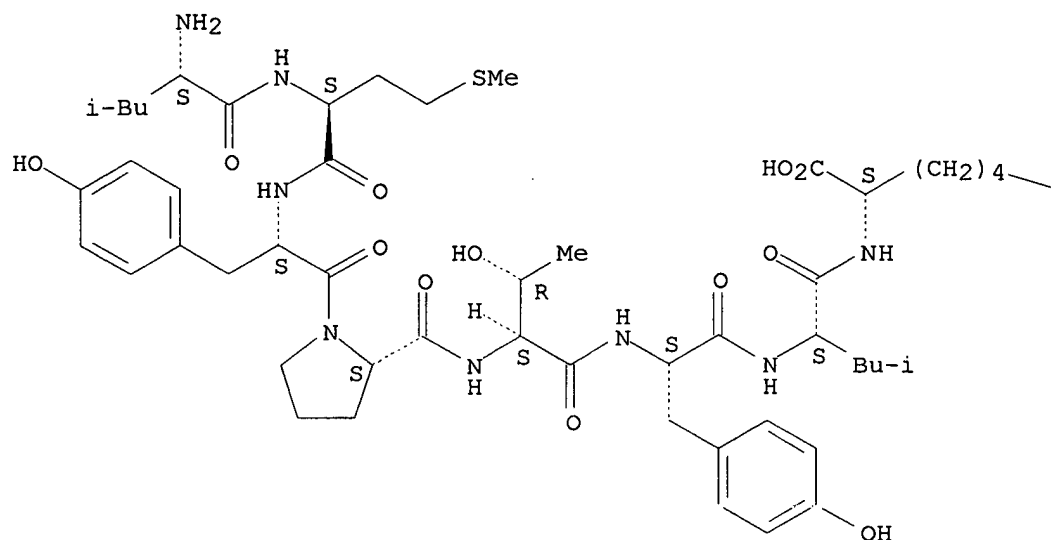
SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXLIT, USPATFULL

Absolute stereochemistry.

Point of Contact:
Jan Delaval
Librarian-Physical Sciences
CM1 1E01 Tel: 308-4498

PAGE 1-A



PAGE 1-B

—NH₂

4 REFERENCES IN FILE CA (1967 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:217605
 REFERENCE 2: 116:249474
 REFERENCE 3: 114:95463
 REFERENCE 4: 110:206193

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:32:46 ON 05 SEP 2000
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FILE COVERS 1967 - 5 Sep 2000 VOL 133 ISS 11
 FILE LAST UPDATED: 4 Sep 2000 (20000904/ED)

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=> d all tot 122

L22 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2000 ACS

AN 1993:617605 HCAPLUS

DN 119:217605

TI The entire vasoactive intestinal polypeptide molecule is required for the activation of the vasoactive intestinal polypeptide receptor: Functional and binding studies on opossum internal anal sphincter smooth muscle

AU Chakder, Sushanta; Rattan, Satish

CS Dep. Med., Thomas Jefferson Univ., Philadelphia, PA, USA

SO J. Pharmacol. Exp. Ther. (1993), 266(1), 392-9

CODEN: JPETAB; ISSN: 0022-3565

DT Journal

LA English

CC 2-2 (Mammalian Hormones)

AB Because no significant information exists regarding the structure-activity of VIP to gut smooth muscle, the authors performed functional studies in vitro on opossum internal anal sphincter (IAS) smooth muscle strips and supplemented them with binding studies to assess the ability of VIP, its fragments, and analogs to inhibit [¹²⁵I]VIP binding to IAS smooth muscle membranes. Binding of radiolabeled VIP to its receptor was specific, saturable, and time- and temp.-dependent. Of all the substances tested, VIP was the most potent in causing a fall in the resting tension of the IAS and inhibiting [¹²⁵I]VIP binding. VIP 2-28, VIP 10-28 and the putative VIP antagonists [4Cl-D-Phe⁶,Leu¹⁷]VIP (VIP analog) and (N-Ac-Tyr¹,D-Phe²)-growth hormone-releasing factor [GRF] (1-29)-NH₂ (GRF analog) caused significant inhibition of [¹²⁵I]VIP binding, but had only minimal effect on the resting tension of the IAS. VIP 9-18 and VIP 1-12 had neither any significant effect nor inhibition of receptor binding. The rank order of potencies nor inhibition of receptor binding. The rank order of potencies for inhibition of binding was VIP > VIP analog > VIP 10-18 = VIP 2-28 > GRF analog > peptide histidine isoleucine > VIP 9-18. The IC₅₀ values for VIP, VIP analog, VIP 10-28, VIP 2-28, GRF analog, and peptide histidine isoleucine were 9.6 .times. 10⁻⁹, 1.6 .times. 10⁻⁷, 5.5 .times. 10⁻⁷, 6.2 .times. 10⁻⁷, 1.2 .times. 10⁻⁸, and 1.2 .times. 10⁻⁵ M, resp. The full action of VIP is critically dependent upon the integrity of the entire VIP mol. However, only the C-terminal part of the mol. is needed for binding to the receptor. These studies provide previously unknown information on selective VIP receptor antagonists and VIP receptor characterization.

ST VIP receptor activation

IT Molecular structure-biological activity relationship

(digestive tract-relaxing, of VIP analogs and fragments)

IT Digestive tract

(relaxation of smooth muscles of, by VIP analogs and fragments, structure in relation to)

IT Receptors

RL: BIOL (Biological study)

(vasoactive intestinal polypeptide, VIP analogs and fragments binding by, structure in relation to)

IT Molecular structure-biological activity relationship

(vasoactive intestinal polypeptide receptor-binding, of VIP analogs and fragments)

IT 40077-57-4, Vasoactive intestinal octacosapeptide (pig) 69856-17-3
 80458-29-3, PHI-27 91409-16-4, VIP-2-28 93965-89-0 102805-45-8
120550-85-8 120928-03-2, VIP-1-12 150503-16-5, VIP-9-18
 RL: BIOL (Biological study)
 (digestive tract smooth muscle relaxation by and receptor binding of,
 structure in relation to)

L22 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2000 ACS

AN 1992:249474 HCAPLUS

DN 116:249474

TI Vasoactive intestinal polypeptide peptide antagonists

IN Gozes, Illana; Brennenman, Douglas; Fridkin, Mati; Moody, Terry

PA United States Dept. of Health and Human Services, USA

SO U. S. Pat. Appl., 35 pp. Avail. NTIS Order No. PAT-APPL-7-620,410.

CODEN: XAXXAV

DT Patent

LA English

CC 2-6 (Mammalian Hormones)

Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 620410	A0	19920215	US 1990-620410	19901130
	US 5217953	A	19930608		

AB Peptide antagonists of vasoactive intestinal polypeptide (VIP) are disclosed. The octomer Leu-Met-Tyr-Pro-Thr-Tyr-Leu-Lys, as well as a VIP-neurotensin hybrid, inhibited VIP-stimulated sexual behavior in rats. The VIP-neurotensin hybrid antagonist was tested for ability to inhibit nonsmall cell lung cancer cell lines; this antagonist inhibited colony formation of cell lines NCI-H522 and NCI-H838, but not NCI-H1246.

ST vasoactive intestinal polypeptide peptide antagonist; neurotensin VIP hybrid VIP antagonist; lung cancer inhibitor VIP antagonist

IT Sexual behavior

(vasoactive intestinal polypeptide antagonist effect on vasoactive intestinal polypeptide-induced, in rat)

IT Peptides, biological studies

RL: BIOL (Biological study)

(vasoactive intestinal polypeptide antagonists)

IT Neoplasm inhibitors

(lung non-small-cell carcinoma, vasoactive intestinal polypeptide-neurotensin hybrid)

IT Lung, neoplasm

(non-small-cell carcinoma, inhibitors, vasoactive intestinal polypeptide-neurotensin hybrid)

IT Receptors

RL: BIOL (Biological study)

(vasoactive intestinal polypeptide, in lung cancer cell lines, vasoactive intestinal polypeptide binding to, vasoactive intestinal polypeptide antagonist activity in relation to)

IT 39379-15-2D, Neurotensin, vasoactive intestinal polypeptide hybrids

RL: BIOL (Biological study)

(as vasoactive intestinal polypeptide antagonist)

IT 37221-79-7, Vasoactive intestinal polypeptide

RL: BIOL (Biological study)

(peptide antagonists of)

IT **120550-85-8**

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(vasoactive intestinal polypeptide antagonist activity of)

L22 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2000 ACS

AN 1991:95463 HCAPLUS

DN 114:95463

TI High affinity receptors for vasoactive intestinal peptide on a human glioma cell line

AU Nielsen, Finn C.; Gammeltoft, Steen; Westermark, Bengt; Fahrenkrug, Jan

Seq ID 3

CS Dep. Clin. Chem., Bispebjerg Hosp., Copenhagen, DK-2400, Den.
 SO Peptides (Fayetteville, N. Y.) (1990), 11(6), 1225-31
 CODEN: PPTDD5; ISSN: 0196-9781
 DT Journal
 LA English
 CC 2-6 (Mammalian Hormones)
 AB VIP bound with high affinity (Kd 0.13 nmol/L) to receptors on the human glioma cell line U-343 MG Cl 2:6. The receptors bound the related peptides helodermin, PHM, and secretin with 10, 400 and 5000 times lower affinity, resp. Deamidated VIP (VIP-COOH) and [des-His1]VIP bound with 10 and 100 times lower affinity. The fragment VIP(7-28) displaced 25% of the receptor-bound 125I-VIP whereas VIP(16-28) and VIP(1-22-NH2) were inactive. The binding of 125I-VIP could be completely inhibited by 10 .mu.mol/L of the antagonists [N-Ac-Tyr1,D-Phe2]GRF(1-29)-NH2, [pCl-D-Phe6,Leu17]VIP and VIP(10-28); in contrast, the antagonist L-8-K was inactive. Affinity labeling showed that VIP bound to proteins with Mr's of 75 kDa, 66 kDa, and 50 kDa, resp. Following binding, the peptide was rapidly internalized, and at steady-state only 20% of cell-assocd. 125I-VIP was bound to receptors on the cell surface. The internalized 125I-VIP was completely degraded to 125I-tyrosine which was released from the cells. Degradn. of internalized 125I-VIP was reduced by chloroquine, phenantroline, and pepstatin-A. Surface binding and internalization of 125I-VIP was increased 3 times by phenantroline, and pepstatin-A caused a 5 times increased in surface binding. Chloroquine reduced surface-bound 125I-VIP, but caused retention of internalized 125I-VIP.

ST glioma VIP receptor internalization
 IT Neuroglia
 (VIP receptors on human)
 IT Receptors
 RL: PROC (Process)
 (for VIP, on glioma cell line of humans, processing of)
 IT Biological transport
 (internalization, of VIP receptors, by human glioma)
 IT 87171-19-5, VIP(16-28) 132333-38-1, VIP(1-22-amide)
 RL: BIOL (Biological study)
 (VIP binding by receptor in human glioma in presence of)
 IT **120550-85-8**
 RL: BIOL (Biological study)
 (VIP binding by receptor of human glioma in presence of)
 IT 69856-17-3 93965-89-0 102805-45-8
 RL: BIOL (Biological study)
 (VIP binding by receptor on human glioma cell line inhibition by)
 IT 40077-61-0 60703-95-9, VIP-COOH 91409-16-4, [Des-His1]VIP
 RL: PROC (Process)
 (binding of, by VIP receptor of glioma of humans)
 IT 37221-79-7, VIP
 RL: BIOL (Biological study)
 (receptors for, of glioma cell line of humans, processing of)

L22 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2000 ACS
 AN 1989:206193 HCAPLUS
 DN 110:206193
 TI High-affinity receptors for vasoactive intestinal peptide on human myeloma cells
 AU Finch, Rosalynde J.; Sreedharan, Sunil P.; Goetzl, Edward J.
 CS Med. Cent., Univ. California, San Francisco, CA, 94143-0724, USA
 SO J. Immunol. (1989), 142(6), 1977-81
 CODEN: JOIMA3; ISSN: 0022-1767
 DT Journal
 LA English
 CC 2-6 (Mammalian Hormones)
 AB Cultured human myeloma cells of the U266 line and leukemic T cells of the Jurkat line bound synthetic [125I]Tyr10-VIP 1-28 ([125I]VIP1-28) specifically and with an affinity similar to that of neuroendocrine cells. Specific binding reached equil. after 2 h at 22.degree. for both myeloma cells and T cells, attained a max. of 57-71% of total binding, and was

reversed in 1.5-3 h by an excess of nonradioactive VIP1-28. Analyses of the ligand concn.-dependence of binding of [125I]VIP1-28 revealed a mean Kd of 7.6 nM for a mean of 41,207 receptors per myeloma cell and 5.2 nM for 12,266 receptors per T cell. The relative affinity of binding of mast cell-derived VIP10-28 free acid and synthetic analogs suggested differences in specificity between lymphocyte and neuroendocrine receptors. Distinct sets of receptors thus appear to mediate the effects of VIP on functions of both antibody-producing cells and T cells.

ST VIP receptor myeloma cell lymphocyte
 IT Myeloma
 (VIP receptors of human in)
 IT Receptors
 RL: BIOL (Biological study)
 (for VIP, of myeloma cells and T-lymphocytes of humans)
 IT Lymphocyte
 (T-, VIP receptors of human in)
 IT 93965-89-0 115722-31-1 **120550-85-8**
 RL: BIOL (Biological study)
 (VIP binding by receptors of myeloma cells antagonism by)
 IT 37221-79-7, Vasoactive intestinal polypeptide
 RL: BIOL (Biological study)
 (receptors for, of myeloma cells and T-lymphocytes of humans)

=> d his 11-117

(FILE 'HOME' ENTERED AT 08:19:46 ON 05 SEP 2000)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 08:19:57 ON 05 SEP 2000

L1 251 S E3-E7,E18
 E MUKHERJEE R/AU
 L2 9 S E3,E4,E6
 E JAGGI M/AU
 L3 605 S E3-E39
 E PRASAD S/AU
 L4 9 S E4
 E PRASAD SUDHAN/AU
 L5 5 S E4-E5,E7,E8
 L6 875 S L1-L5
 L7 6 S L6 AND 34/SC,SX
 L8 17 S L6 AND ?PEPTIDE?
 L9 0 S L6 AND BOMBESIN
 L10 2 S L6 AND DXG
 L11 2 S L10 AND L7,L8
 L12 2 S L1 AND L2-L5
 L13 1 S L2 AND L3-L5
 L14 1 S L3,L4 AND L5
 L15 2 S L12-L14
 L16 1 S L15 AND 63/SC,SX
 L17 3 S L11,L16

=> d all tot 117

L17 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2000 ACS
 AN 2000:573679 HCAPLUS
 TI Antiangiogenic drugs
 IN **Mukherjee, Rama; Jaggi, Manu; Prasad,**
Sudhanand; Burman, Anand C.; Rajendran, Praveen; Mathur,
 Archana; Singh, Anu T.
 PA National Institute of Immunology, India; Dabur Research Foundation; Cord,
 Janet, I.
 SO PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K038-00

ICS A61K038-02; C07K005-00; C07K007-00

CC 63 (Pharmaceuticals)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000047221	A1	20000817	WO 2000-US3559	20000211
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRAI US 1999-248381 19990211

AB The invention relates to the use of peptides individually or in combination, for treating and/or preventing angiogenesis. It also relates to the use of peptide analogs or a combination of peptides referred to as MuJ-7 as anticancer drugs in restricting the tumor growth and spread by inhibiting tumor angiogenesis. MuJ-7, in addition inhibits metastasis through its antiangiogenic activity in all cancers. The invention also relates to a pharmaceutical composition containing either individual peptides or in combination, and methods of treatment of human beings and animals for curing and/or preventing angiogenesis.

RE.CNT 8

RE

- (1) Bogden; US 5217955 A 1993
- (2) Coy; US 5410019 A 1995 HCAPLUS
- (3) Danesi; Metabolism 1996, V45(8, Suppl 1), P49
- (4) Gozes; US 5565424 A 1996
- (5) Hanahan; Cell 1996, V86, P353 HCAPLUS
- (6) Kim; US 5552520 A 1996 HCAPLUS
- (7) The Administrators Of The Tulane Educational Fund; WO 9639161 A1 1996 HCAPLUS
- (8) Woltering; Journal of Surgical Research 1991, V50(3), P245 HCAPLUS

L17 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:678144 HCAPLUS

DN 125:326338

TI Conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2

AU **Prasad, Sudhanand**; Rao, R. Balaji; Bergstrand, Hakan; Lundquist, Britta; Becker, Elmer L.; Balaram, P.

CS Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India

SO Int. J. Pept. Protein Res. (1996), 48(4), 312-318

CODEN: IJPPC3; ISSN: 0367-8377

DT Journal

LA English

CC 15-10 (Immunochemistry)

AB Five stereochem. constrained analogs of the chemotactic **tripeptide** incorporating 1-aminocycloalkane-1-carboxylic acid (Acnc) and .chi.,.chi.-dialkylglycines (Deg, diethylglycine; Dpg, n,n-dipropylglycine and Dbg, n,n-dibutylglycine) at position 2 have been synthesized. NMR studies of **peptides** For-Met-Xxx-Phe-OMe (Xxx=Ac7c I; Ac8c, II; Deg, III; Dpg, IV and Dbg, V; For, formyl) establish that **peptide** with cycloalkyl residues, I and II, adopt folded .beta.-turn conformations in CDC13 and (CD3)2SO. In contrast, analogs with linear alkyl sidechains, III-V, favor fully extended (C5) conformations in soln. **Peptides** I-V exhibit high activity in inducing .beta.-glucosaminidase release from rabbit neutrophils, with ED50

values ranging from 1.4-8.0 x 10⁻¹¹M. In human neutrophils the **Dxg peptides** III-V have ED50 values ranging from 2.3 x 10⁻¹⁰ M, with the activity order being V>IV>III. While **peptides** I-IV are less active than the parent, For-Met-Leu-Phe-OH, in stimulating histamine release from human basophils, the **Dbg peptide** V is appreciably more potent, suggesting its potential utility as a probe for formyl **peptide** receptors.

ST chemotactic **tripeptide** conformation activity correlation

IT Basophil

Neutrophil

(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT **Peptide** receptors

Receptors

RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(1-(N-formylmethionine)-**peptide**, conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT Molecular structure-biological activity relationship

(chemotactic, conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 51-45-6, Histamine, biological studies 9012-33-3

RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 127291-39-8P 136427-57-1P 181701-83-7P 183429-69-8P 183429-77-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 2488-15-5 2577-90-4 6141-45-3 70974-26-4 87113-23-3 183429-63-2
183429-68-7

RL: RCT (Reactant)

(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 138123-33-8P 183429-61-0P 183429-62-1P 183429-65-4P 183429-66-5P
183429-67-6P 183429-70-1P 183429-71-2P 183429-72-3P 183429-74-5P
183429-75-6P 183429-76-7P 183429-78-9P 183429-79-0P 183429-80-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

L17 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2000 ACS

AN 1995:406397 HCAPLUS

DN 122:315080

TI Contrasting solution conformations of **peptides** containing .alpha.,.alpha.-dialkylated residues with linear and cyclic side chains

AU **Prasad, Sudhanand**; Rao, R. Balaji; Balaram, P.

CS Dep. Chem., Banaras Hindu Univ., Varanasi, 221 005, India

SO Biopolymers (1995), 35(1), 11-20

CODEN: BIPMAA; ISSN: 0006-3525

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 22

AB The conformational properties of five **peptides** Boc-Ala-X-Ala-OMe

[Boc = Me₃CO₂C; X = diethylglycine (I), dipropylglycine (II), dibutylglycine (III), 1-aminocyclohexane-1-carboxylic acid (IV), and 1-aminocycloheptane-1-carboxylic acid (V)] contg. acyclic .alpha.,.alpha.-dialkylglycine (**Dxg**) and 1-aminocycloalkane-1-carboxylic acid (Acnc) residues were studied in soln. by NMR and CD.

Delineation of solvent-shielded NH groups have been achieved by solvent and temp. dependence of NH chem. shifts in CDCl₃ and (CD₃)₂SO and by paramagnetic radical induced line broadening in **peptide** III. In **Dxg**-contg. **peptides** I-III, the order of solvent exposure of NH groups is Ala1 > Ala3 > Dxg2, whereas in Acnc-contg. **peptides** IV and V, the order of solvent exposure of NH groups is Ala1 > Acnc2 > Ala3. The NMR results suggest that Acnc-contg. **peptides** IV and V adopt folded .beta.-turn conformations with Ala1 and Acnc2 occupying i + 1 and i + 2 positions. In contrast, **Dxg**-contg. **peptides** I-III favor extended C5 conformations. The conformational differences in the two series are clearly borne out in CD studies. The soln. conformations of **Dxg**-contg. **peptides** I-III are distinctly different from the .beta.-turn structure obsd. in crystals. Low temp. NMR spectra recorded immediately after dissoln. of crystals of **peptide** II provide evidence for a structural transition. Introduction of an addnl. hydrogen-bonding function in Boc-Ala-Dpg-Ala-NHMe (VI) results in a stabilization of a consecutive .beta.-turn or incipient 310-helix in soln.

- ST conformation dialkylated amino acid **peptide**;
aminocycloalkanecarboxylic acid **peptide** conformation; glycine
dialkyl **peptide** conformation
- IT Conformation and Conformers
(contrasting soln. conformations of **peptides** contg.
.alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid
residues)
- IT **Peptides**, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(dialkylglycine-contg.; contrasting soln. conformations of
peptides contg. .alpha.,.alpha.-dialkylglycine and
aminocycloalkanecarboxylic acid residues)
- IT **Peptides**, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(aminocycloalkanecarboxylic acid-contg., contrasting soln.
conformations of **peptides** contg. .alpha.,.alpha.-
dialkylglycine and aminocycloalkanecarboxylic acid residues)
- IT 163493-04-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation)
(contrasting soln. conformations of **peptides** contg.
.alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid
residues)
- IT 163493-05-8P 163493-06-9P 163493-17-2P 163493-18-3P 163493-19-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(contrasting soln. conformations of **peptides** contg.
.alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid
residues)
- IT 96-22-0, 3-Pentanone 108-94-1, Cyclohexanone, reactions 123-19-3,
4-Heptanone 502-42-1, Cycloheptanone 502-56-7, 5-Nonanone 2491-20-5,
Alanine methyl ester hydrochloride 15761-38-3
RL: RCT (Reactant)
(contrasting soln. conformations of **peptides** contg.
.alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid
residues)
- IT 702-62-5P, 1,3-Diazaspiro[4.5]decane-2,4-dione 707-16-4P,
1,3-Diazaspiro[4.6]undecane-2,4-dione 2566-29-2P, .alpha.,.alpha.-
Diethylglycine 2566-31-6P, .alpha.,.alpha.-Dipropylglycine 2756-85-6P,
1-Aminocyclohexane-1-carboxylic acid 5455-34-5P, 5,5-Diethylhydantoin
6141-45-3P 6949-77-5P, 1-Aminocycloheptane-1-carboxylic acid
7148-46-1P, 2,4-Imidazolidinedione, 5,5-dibutyl- 7597-66-2P,
.alpha.,.alpha.-Dibutylglycine 36033-33-7P 37993-32-1P 87113-23-3P
92398-50-0P 92398-54-4P 163493-07-0P 163493-08-1P 163493-09-2P
163493-10-5P 163493-11-6P 163493-12-7P 163493-13-8P 163493-14-9P
163493-15-0P 163493-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(contrasting soln. conformations of **peptides** contg.
.alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid

residues)

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:25:04 ON 05 SEP 2000
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2000 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 4 SEP 2000 HIGHEST RN 288141-13-9
 DICTIONARY FILE UPDATES: 4 SEP 2000 HIGHEST RN 288141-13-9

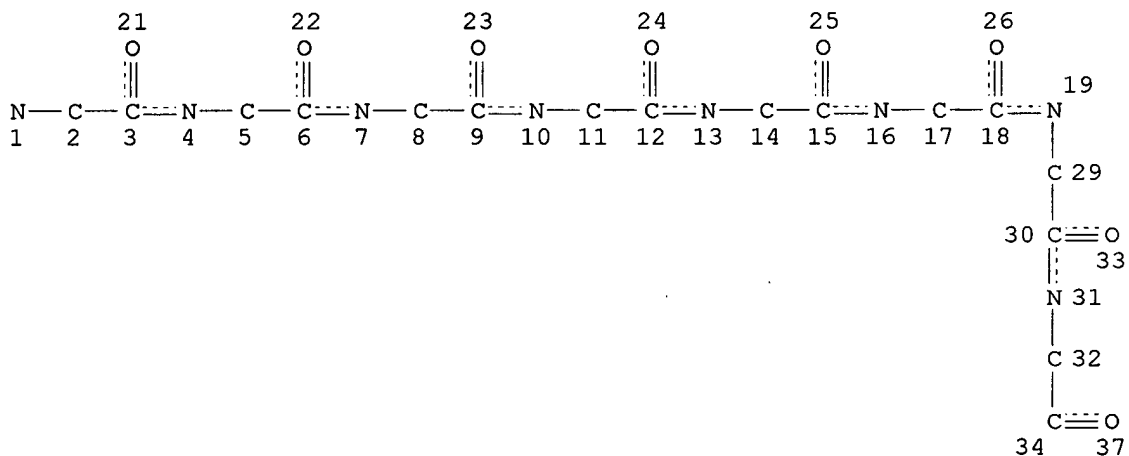
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT
 for details.

=> d sta que 164

L28 27670 SEA FILE=REGISTRY ABB=ON PLU=ON PROTEIN/FS AND 8/SQL
 L30 STR



NODE ATTRIBUTES:

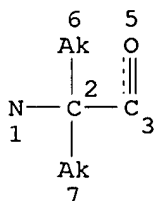
NSPEC IS RC AT 2
 NSPEC IS RC AT 5
 NSPEC IS RC AT 8
 NSPEC IS RC AT 11
 NSPEC IS RC AT 14
 NSPEC IS RC AT 17
 NSPEC IS RC AT 29
 NSPEC IS RC AT 32
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

L32 10689 SEA FILE=REGISTRY SUB=L28 SSS FUL L30
 L33 STR



NODE ATTRIBUTES:

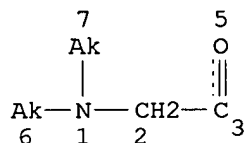
CONNECT IS E1 RC AT 6
 CONNECT IS E1 RC AT 7
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

L34 STR



NODE ATTRIBUTES:

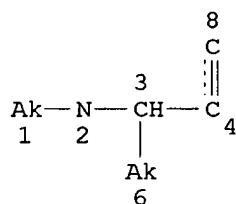
CONNECT IS E1 RC AT 6
 CONNECT IS E1 RC AT 7
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

L35 STR



NODE ATTRIBUTES:

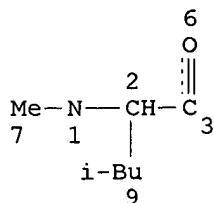
CONNECT IS E1 RC AT 1
 CONNECT IS E1 RC AT 6
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

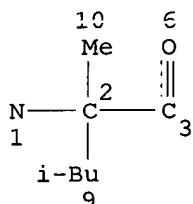
L36 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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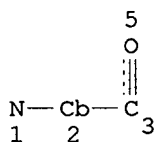
STEREO ATTRIBUTES: NONE
 L37 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
 L38 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L40 244 SEA FILE=REGISTRY SUB=L32 SSS FUL (L33 OR L34 OR L35 OR L36 OR L37 OR L38)
 L48 26 SEA FILE=REGISTRY ABB=ON PLU=ON (174350-44-8/BI OR 135013-53-5/BI OR 135013-54-6/BI OR 188064-10-0/BI OR 188064-21-3/BI OR 188064-25-7/BI OR 188064-27-9/BI OR 188064-28-0/BI OR 188064-30-4/BI OR 188064-32-6/BI OR 189098-41-7/BI OR 189098-42-8/BI OR 189098-43-9/BI OR 189098-44-0/BI OR 189098-45-1/BI OR 201984-90-9/BI OR 201984-94-3/BI OR 201984-95-4/BI OR 201984-99-8/BI OR 201985-00-4/BI OR 220331-94-2/BI OR 220332-02-5/BI OR 259107-45-4/BI OR 259107-49-8/BI OR 259107-50-1/BI OR 259107-54-5/BI)
 L49 218 SEA FILE=REGISTRY ABB=ON PLU=ON L40 NOT L48

L50 10 SEA FILE=REGISTRY ABB=ON PLU=ON L49 AND (C3 OR C4 OR C5 OR
 C7 OR C8)/ES
 L52 2 SEA FILE=REGISTRY ABB=ON PLU=ON L50 AND (C35H47N9O9 OR
 C50H88N8O11)
 L53 186 SEA FILE=REGISTRY ABB=ON PLU=ON L49 NOT (NC4-C6 OR NCNC2)/ES
 L54 184 SEA FILE=REGISTRY ABB=ON PLU=ON L53 NOT L50
 L55 124 SEA FILE=REGISTRY ABB=ON PLU=ON L54 AND 46.150.18/RID
 L56 60 SEA FILE=REGISTRY ABB=ON PLU=ON L54 NOT L55
 L57 14 SEA FILE=REGISTRY ABB=ON PLU=ON L56 AND NR>=1
 L58 46 SEA FILE=REGISTRY ABB=ON PLU=ON L56 NOT L57
 L59 9 SEA FILE=REGISTRY ABB=ON PLU=ON L58 AND (C28H50N8O9 OR
 C29H52N8O9 OR C33H60N8O9 OR C32H62N8O9 OR C31H56N8O9 OR
 C34H62N8O9 OR C48H90N8O9 OR C32H58N8O9 OR C49H92N8O9)
 L64 11 SEA FILE=REGISTRY ABB=ON PLU=ON (L52 OR L59)

=> d sqide can tot l64

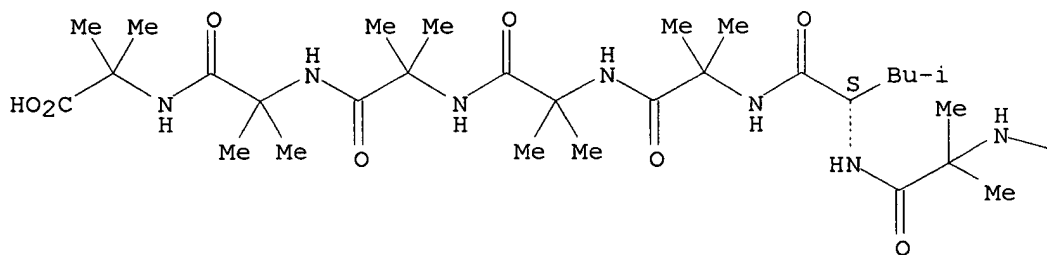
L64 ANSWER 1 OF 11 REGISTRY COPYRIGHT 2000 ACS
 RN 281664-71-9 REGISTRY
 CN Alanine, 2-methylalanyl-2-methylalanyl-L-leucyl-2-methylalanyl-2-
 methylalanyl-2-methylalanyl-2-methylalanyl-2-methyl- (9CI) (CA INDEX
 NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 SQL 8
 NTE

type	location			description
uncommon	Aib-1	-	-	
uncommon	Aib-2	-	-	
uncommon	Aib-4	-	-	
uncommon	Aib-5	-	-	
uncommon	Aib-6	-	-	
uncommon	Aib-7	-	-	
uncommon	Aib-8	-	-	

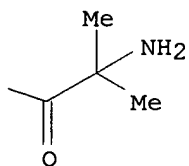
SEQ 1 XXLXXXXX
 MF C34 H62 N8 O9
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

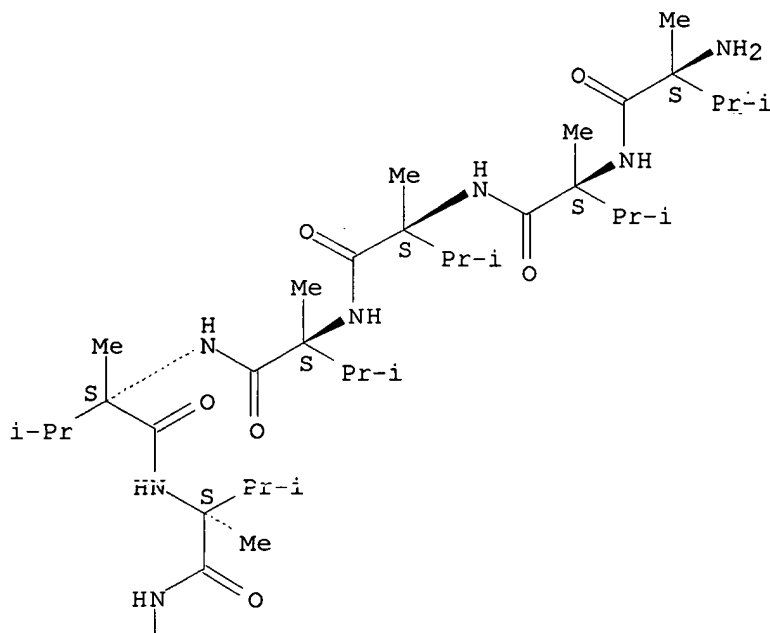
PAGE 1-A



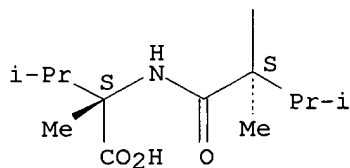
PAGE 1-B



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PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:89770

L64 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2000 ACS

RN 223617-32-1 REGISTRY

CN 4-10-Trikonigin KB I, 10-L-isoleucine-10a-L-leucine-, methyl ester (9CI)
(CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 8

NTE modified

type	----- location -----	description
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uncommon	Aib-5 - -	

SEQ 1 XGGVXGIL

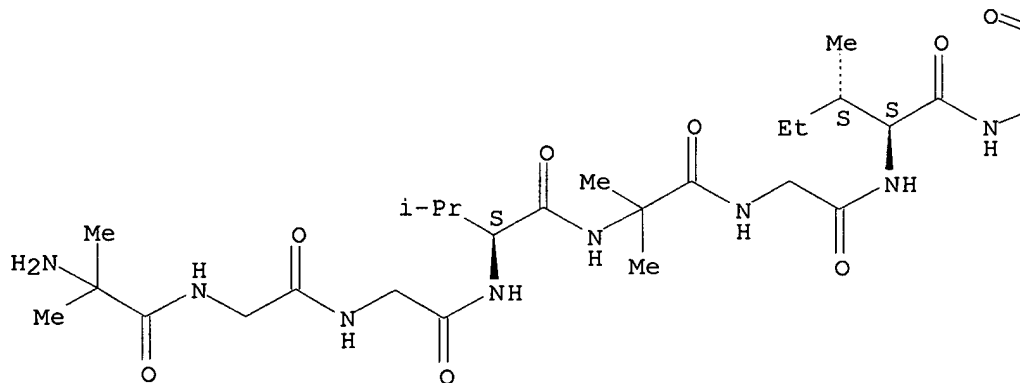
MF C32 H58 N8 O9

SR CA

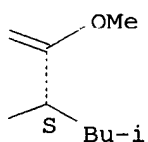
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:312066

L64 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2000 ACS

RN 214058-85-2 REGISTRY

CN Cyclopropanecarboxamide, 1-[[[1-[[[1-[[[1-[[[1-(acetylamino)cyclopropyl]carbonyl]amino]cyclopropyl]carbonyl]amino]cyclopropyl]carbonyl]amino]cyclopropyl]carbonyl]amino]-N-[1-[[[1-[[[1-(methylamino)carbonyl]cyclopropyl]amino]carbonyl]cyclopropyl]amino]carbonyl]cyclopropyl]- (9CI) (CA INDEX NAME)

FS	PROTEIN	SEQUENCE
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2	2	2
3	3	3
4	4	4
5	5	5
6	6	6
7	7	7
8	8	8
9	9	9
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100	100	100

SOL 8

NTE modified (modifications unspecified)

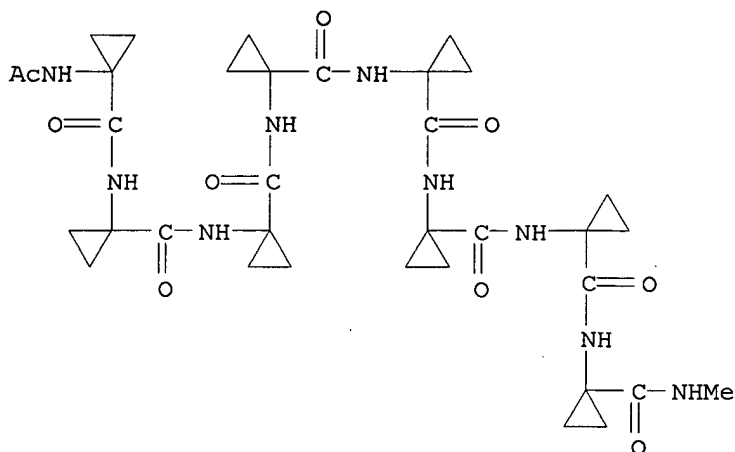
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uncommon	Aaa-3	-	-
uncommon	Aaa-4	-	-
uncommon	Aaa-5	-	-
uncommon	Aaa-6	-	-
uncommon	Aaa-7	-	-
uncommon	Aaa-8	-	-

```
SEQ      1  XXXXXXXXX
```

MF C35 H47 N9 O9

SR CA

LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:276333

L64 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2000 ACS

RN 183667-57-4 REGISTRY

CN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-1-aminocyclooctanecarbonyl-L-valylglycylglycyl-L-leucyl-1-aminocyclooctanecarbonyl-, methyl ester (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 8

NTE modified (modifications unspecified)

type	-----	location	-----	description
uncommon	Aaa-2	-	-	
uncommon	Aaa-7	-	-	

SEQ 1 LXVGGLXV

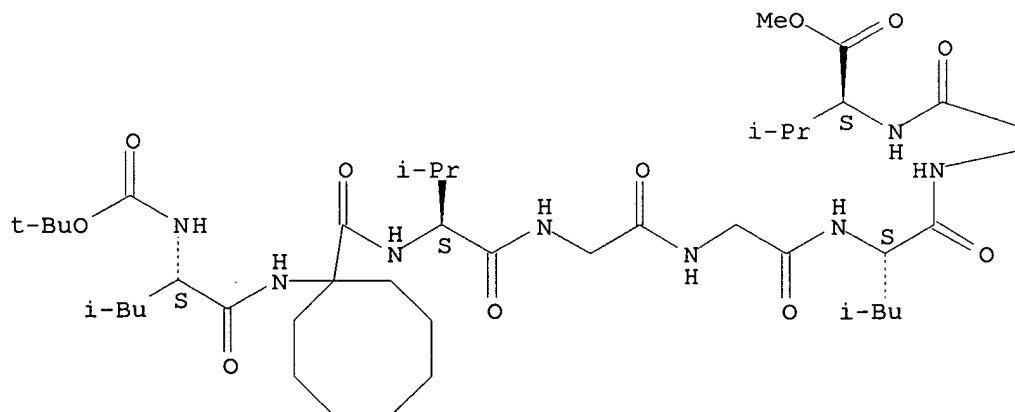
MF C50 H88 N8 O11

SR CA

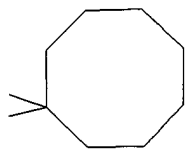
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:320867

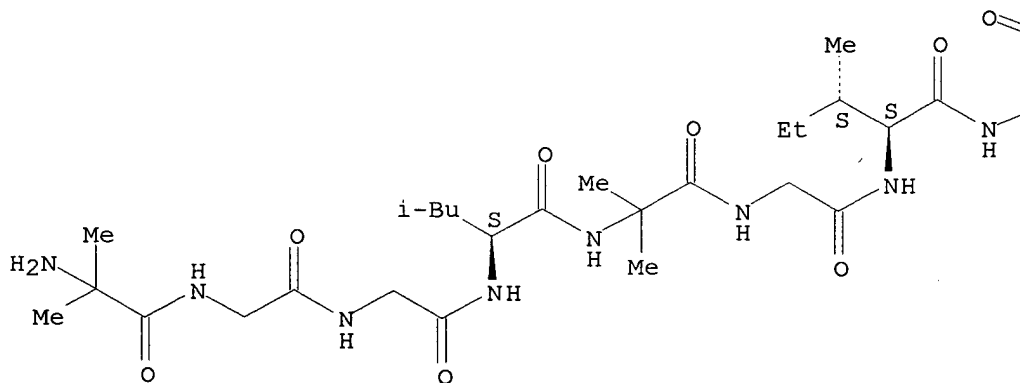
L64 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2000 ACS
 RN 176664-81-6 REGISTRY
 CN 4-10-Trichogin A IV, 9-L-isoleucine-10a-L-leucine-, methyl ester (9CI)
 (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 SQL 8
 NTE modified

type	location			description
uncommon	Aib-1	-	-	
uncommon	Aib-5	-	-	

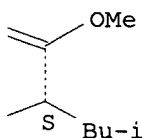
SEQ 1 XGGLXGIL
 MF C33 H60 N8 O9
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:336177

L64 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2000 ACS

RN 148505-60-6 REGISTRY

CN Alanine, N-[N-[N-[N-[N-(N-L-alanyl-2-methylalanyl)-L-alanyl]-2-methylalanyl]-L-alanyl]-2-methylalanyl]-L-alanyl]-2-methyl-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 8

NTE modified

type	location	description
uncommon	Aib-2	-
uncommon	Aib-4	-
uncommon	Aib-6	-
uncommon	Aib-8	-
modification	-	undetermined modification

SEQ 1 AXAXAXAX

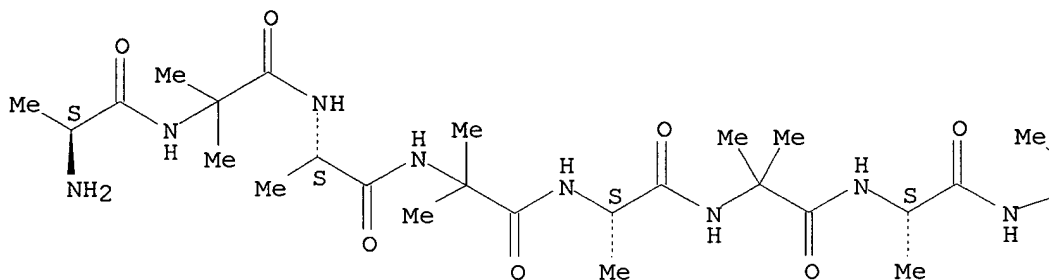
MF C29 H52 N8 O9 . C1 H

SR CA

LC STN Files: CA, CAPLUS

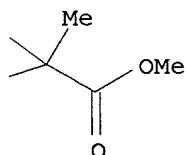
Absolute stereochemistry.

PAGE 1-A



● HCl

PAGE 1-B



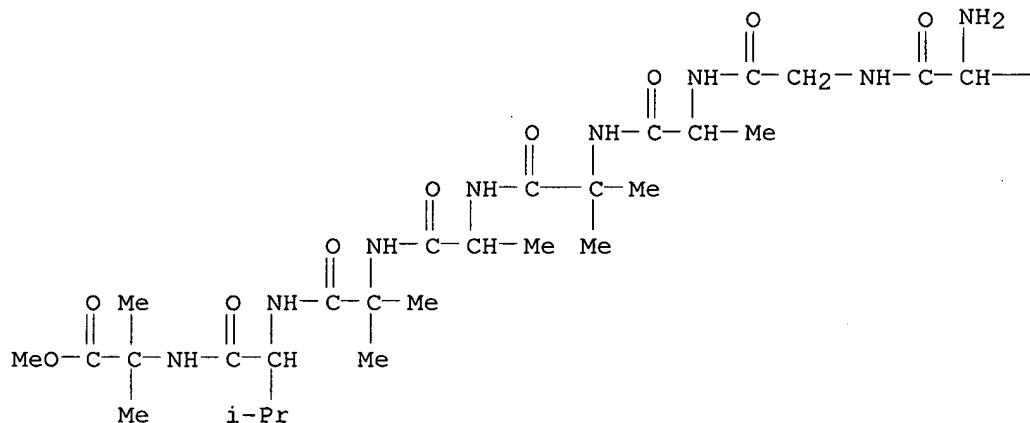
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:43723

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uncommon	Aib-6	-	-	
uncommon	Aib-8	-	-	
modification	-	-		undetermined modification

PAGE 1-A



● HCl

PAGE 1-B

— Pr-i

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 117:172078

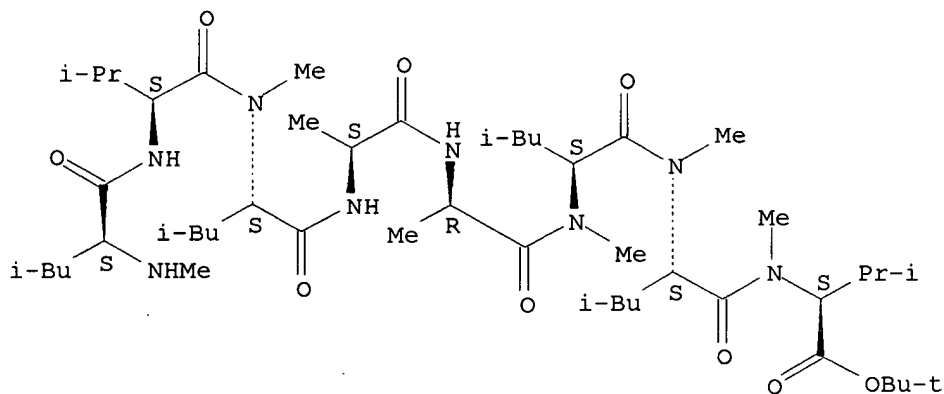
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L64  ANSWER 9 OF 11  REGISTRY  COPYRIGHT 2000 ACS
RN   117106-24-8  REGISTRY
CN   L-Valine, N-methyl-N-[N-methyl-N-[N-methyl-N-[N-[N-methyl-N-[N-(N-
methyl-L-leucyl)-L-valyl]-L-leucyl]-L-alanyl]-D-alanyl]-L-leucyl]-L-
leucyl]-, 1,1-dimethylethyl ester (9CI)  (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
```

SQL 8
NTE modified

type	location		description
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modification	Leu-3	-	methyl<Me>
modification	Leu-6	-	methyl<Me>
modification	Leu-7	-	methyl<Me>
modification	Val-8	-	methyl<Me>

SEQ 1 LVLAALLV
MF C49 H92 N8 O9
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:190816

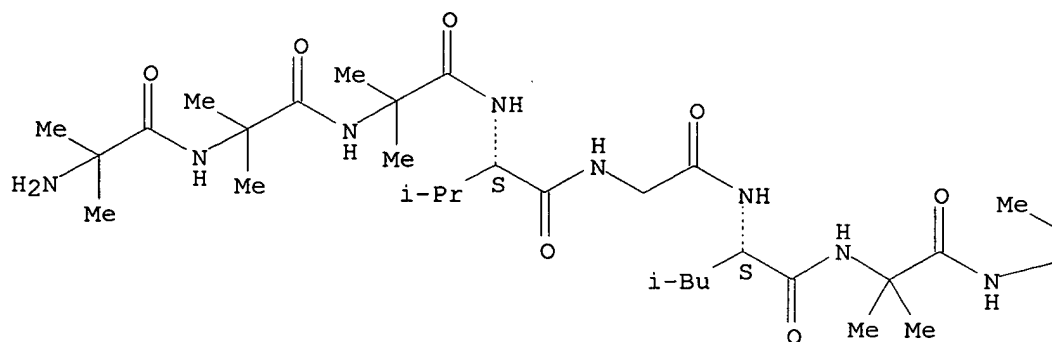
L64 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 100843-78-5 REGISTRY
CN Alanine, 2-methyl-N-[2-methyl-N-[N-[N-[N-[2-methyl-N-[2-methyl-N-(2-methylalanyl)alanyl]alanyl]-L-valyl]glycyl]-L-leucyl]alanyl]-, methyl ester (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified

type	location		description
uncommon	Aib-1	-	-
uncommon	Aib-2	-	-
uncommon	Aib-3	-	-
uncommon	Aib-7	-	-
uncommon	Aib-8	-	-

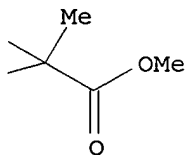
SEQ 1 XXXVGLXX
MF C34 H62 N8 O9
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 104:104617

L64 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2000 ACS

RN 70134-43-9 REGISTRY

CN L-Alanine, N-[2-methyl-N-[N-[2-methyl-N-[N-[2-methyl-N-[N-(2-methylalanyl)-L-alanyl]alanyl]-L-alanyl]alanyl]-L-alanyl]alanyl]- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 8

NTE

type	----- location -----	description
uncommon	Aib-1 - -	
uncommon	Aib-3 - -	
uncommon	Aib-5 - -	
uncommon	Aib-7 - -	

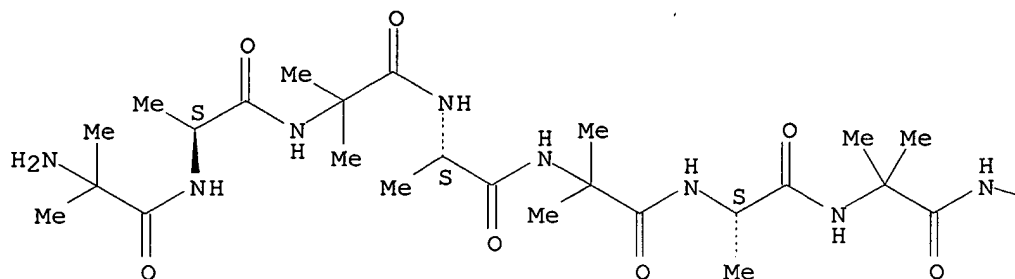
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MF C28 H50 N8 O9

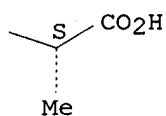
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:187312

=> d his 164-

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 SAV L64 MOEZIE248B/A

FILE 'HCAOLD' ENTERED AT 09:24:50 ON 05 SEP 2000
 L65 0 S L64

FILE 'HCAPLUS' ENTERED AT 09:24:57 ON 05 SEP 2000
 L66 10 S L64

FILE 'REGISTRY' ENTERED AT 09:25:04 ON 05 SEP 2000

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 09:25:19 ON 05 SEP 2000
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FILE COVERS 1967 - 5 Sep 2000 VOL 133 ISS 11
 FILE LAST UPDATED: 4 Sep 2000 (20000904/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in HCAPLUS on STN.

=> d all tot 166

L66 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:211479 HCAPLUS
DN 133:89770
TI Simulations of oligopeptide vibrational CD: effects of isotopic labeling
AU Bour, Petr; Kubelka, Jan; Keiderling, Timothy A.
CS Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.
SO Biopolymers (2000), 53(5), 380-395
CODEN: BIPMAA; ISSN: 0006-3525
PB John Wiley & Sons, Inc.
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22
AB Simulated IR absorption and vibrational CD (VCD) spectra of alanine-based octapeptides, each having its main chain constrained to a different secondary structure conformation (.alpha.-helix, 310-helix, ProII-like helix and .beta.-sheet-like strand), were analyzed and compared with exptl. results for several different peptides. The octapeptide simulations were based on transfer of property tensors from a series of ab initio calcns. for a short L-alanine based segment contg. 3 peptide bonds with relative .phi., .psi. angles fixed to those appropriate for .alpha.-helix, 310-helix, ProII-like helix, and .beta.-sheet-like strand. The tripeptide force field (FF) and at. polar tensors were obtained with d. functional theory techniques at the BPW91/6-31G** level and the at. axial tensor at the mixed BPW91/6-31G**/HF/6-31G level. Allowing for frequency correction due to the FF limitations, the octapeptide results obtained are qual. consistent with exptl. observations for IR and VCD spectra of polypeptides and oligopeptides in established conformations. In all cases, the correct VCD sign patterns for the amide I and II bands were predicted, but the intensities did have some variation from the exptl. patterns. Predicted VCD changes upon deuteration of either the peptide or side-chains as well as for 13C isotopic labeling of the amide C:O at specific sites in the peptide chain were computed for anal. of exptl. observations. A combination of theor. modeling with exptl. data for labeled compds. leads both to enhanced resoln. of component transitions and added conformational applicability of the VCD spectra.
ST alanine octapeptide vibrational CD simulation isotope labeling effect; secondary structure conformation simulated alanine octapeptide
IT Helix (conformation)
(310-helical; calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
IT Immunoglobulins
RL: PRP (Properties)
(G; exptl. vibrational CD data for comparing with the computed vibrational CD of model alanine octapeptide)
IT Ab initio methods
Conformation
Simulation and Modeling, physicochemical
.alpha.-Helix
.beta.-Sheet

- (calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
- IT Isotope effect
Secondary structure
Vibrational circular dichroism
(effect of isotopic labeling on simulated vibrational CD spectra for the model alanine octapeptide)
- IT Peptides, properties
RL: PRP (Properties)
(oligopeptides; calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
- IT Conformation
(.beta.-turn, type II; effect of isotopic labeling on simulated vibrational CD spectra for the model alanine octapeptide)
- IT 128371-85-7
RL: PRP (Properties)
(calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
- IT 281664-72-0 281664-73-1 281664-74-2 281664-75-3
RL: PRP (Properties)
(effect of isotopic labeling on simulated vibrational CD spectra for the model alanine octapeptide)
- IT 21379-66-8 25014-27-1, Poly-.gamma.-benzyl-L-Glutamate 25038-53-3
25104-18-1, Poly(L-lysine) 38000-06-5, Poly(L-lysine), SRU 64809-02-5
64809-10-5 281664-68-4 **281664-70-8 281664-71-9**
RL: PRP (Properties)
(exptl. vibrational CD data for comparing with the computed vibrational CD of model alanine octapeptide)
- IT 27482-45-7
RL: PRP (Properties)
(simulated vibrational CD spectra for the model pseudo-alanine-tripeptide)

RE.CNT 98

RE

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- L66 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2000 ACS
 AN 1999:187356 HCAPLUS
 DN 130:312066
 TI Total synthesis and membrane modifying properties of the lipopeptaibol
 Trikoningin KB II and its analogs with acyl chains of different length at
 the N- and C-termini
 AU Piazza, Claudia; Formaggio, Fernando; Crisma, Marco; Toniolo, Claudio;
 Kamphuis, Johan; Kaptein, Bernard; Broxterman, Quirinus B.
 CS Department of Organic Chemistry, Biopolymer Research Centre, C.N.R.,
 University of Padova, Padua, 35131, Italy
 SO J. Pept. Sci. (1999), 5(2), 96-102
 CODEN: JPSIEI; ISSN: 1075-2617
 PB John Wiley & Sons Ltd.
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1
 AB Trikoningin KB II, a ten-amino acid residue lipopeptaibol blocked at the
 N-terminus by the n-octanoyl group and at the C-terminus by the 1,2-amino
 alc. L-leucinol, and extd. from the fungus *Trichoderma koningii*, exhibits
 membrane-modifying properties. The authors have synthesized by
 soln.-phase methods trikoningin KB II and several analogs with acyl chains
 of different length at the N- and C-termini. Lipopeptaibols bind to
 phospholipid bilayers and are able to modify their permeability.
 Therefore, the permeability properties of trikoningin KB II and its
 analogs with acyl chains of different length at the N- and C-termini were
 investigated by following fluorimetrically the induced CF leakage from
 small unilamellar vesicles (egg PC-cholesterol 70:30) for different Rt-1 =
 [peptide]/[lipid] molar ratios. Permeability measurements showed that an
 appropriate length of the linear acyl chain is a more important
 characteristic for the onset of significant membrane-modifying activity
 than its position in the peptide chain. New relevant information extd.
 from this work may be summarized as follows: (i) in striking contrast to
 the effect produced by one long (C8) acyl chain, two short (C4) acyl
 chains, each with half no. of carbon atoms, concomitantly linked at the
 two termini of the peptide chain, are not able to induce any appreciable
 membrane activity; (ii) the position of the long acyl chain does have some
 influence, albeit not dramatic, on membrane activity (it is higher when
 the C8 acyl chain is located at the N-terminus of the peptide chain);
 (iii) the presence of two C8 acyl chains, concomitantly linked at the two
 termini of the peptide chain, produces a significant increase in membrane
 activity.
 ST lipopeptaibol trikoningin KB II analog prepn membrane modifying activity;
 peptide prepn acyl chain length membrane; permeability membrane
 trikoningin KB II analog
 IT Cell membrane
 Membranes (biological)
 Permeability
 (total synthesis and membrane modifying properties of lipopeptaibol
 Trikoningin KB II and its analogs with acyl chains of different length
 at N- and C-termini)
 IT Peptides, preparation
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation)
 (total synthesis and membrane modifying properties of lipopeptaibol
 Trikoningin KB II and its analogs with acyl chains of different length
 at N- and C-termini)
 IT 223616-71-5P 223616-75-9P 223616-77-1P 223616-79-3P 223616-82-8P
 223616-86-2P 223616-90-8P 223616-92-0P 223616-94-2P
 RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(total synthesis and membrane modifying properties of lipopeptaibol
 Trikoningin KB II and its analogs with acyl chains of different length
 at N- and C-termini)

IT 1138-80-3 1149-26-4 2666-93-5 3160-59-6 15030-72-5 163312-63-8,
 Z-D-Iva-OH

RL: RCT (Reactant)

(total synthesis and membrane modifying properties of lipopeptaibol
 Trikoningin KB II and its analogs with acyl chains of different length
 at N- and C-termini)

IT 4818-03-5P 15030-74-7P, (Z-Aib)2O 54793-59-8P 119768-28-4P
 156916-67-5P 164575-77-3P 176664-73-6P 223616-46-4P 223616-49-7P
 223616-53-3P 223616-57-7P 223616-61-3P 223616-65-7P 223616-67-9P
 223617-15-0P 223617-22-9P 223617-28-5P **223617-32-1P**
 223617-35-4P 223617-38-7P 223617-42-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(total synthesis and membrane modifying properties of lipopeptaibol
 Trikoningin KB II and its analogs with acyl chains of different length
 at N- and C-termini)

RE.CNT 30

RE

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L66 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1998:590250 HCAPLUS

DN 129:276333

TI PAPQMD parametrization of molecular systems with cyclopropyl rings:
 conformational study of homopeptides constituted by 1-aminocyclopropane-1-
 carboxylic acid

AU Aleman, Carlos; Casanovas, Jordi; Galembeck, Sergio E.

CS Departament d'Enginyeria Quimica, Universitat Politecnica de Catalunya,
 Barcelona, E-08028, Spain

SO J. Comput.-Aided Mol. Des. (1998), 12(3), 259-273

CODEN: JCADEQ; ISSN: 0920-654X

PB Kluwer Academic Publishers

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 22

- AB The suitability of ab initio, semiempirical and d. functional methods as sources of stretching and bending parameters has been explored using the PAPQMD (program for approx. parametrization from quantum mech. data) strategy. Results show that semiempirical methods provide parameters comparable to those compiled on empirical force fields. In this respect the AM1 method seems to be a good method to obtain parameters at a min. computational cost. On the other hand, harmonic force fields initially developed for proteins and DNA have been extended to include compds. contg. highly strained three-membered rings, like 1-aminocyclopropane-1-carboxylic acid. For this purpose the cyclopropyl ring has been explicitly parametrized at the AM1 level considering different chem. environments. Finally, the new set of parameters has been used to investigate the conformational preferences of homopeptides constituted by 1-aminocyclopropane-1-carboxylic acid. Results indicate that such compds. tend to adopt a helical conformation stabilized by intramol. hydrogen bonds between residues i and i + 3. This conformation allows the arrangement of the cyclic side chains without steric clashes.
- ST aminocyclopropanecarboxylic acid homopeptide conformation PAPQMD parametrization; AM1 MO aminocyclopropanecarboxylic acid homopeptide conformation
- IT AM1 MO (molecular orbital)
Conformation
(PAPQMD parametrization of mol. systems with cyclopropyl rings and conformational study of aminocyclopropanecarboxylic acid homopeptides)
- IT Peptides, properties
RL: PRP (Properties)
(aminocyclopropanecarboxylic acid-contg.; PAPQMD parametrization of mol. systems with cyclopropyl rings and conformational study of aminocyclopropanecarboxylic acid homopeptides)
- IT 75-19-4, Cyclopropane 22059-21-8, 1-Aminocyclopropane-1-carboxylic acid 99451-23-7 126705-26-8 129618-40-2, Nevirapine 214058-82-9 214058-83-0 **214058-85-2** 214058-86-3 214058-87-4
RL: PRP (Properties)
(PAPQMD parametrization of mol. systems with cyclopropyl rings and conformational study of aminocyclopropanecarboxylic acid homopeptides)

L66 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:701427 HCAPLUS

DN 125:320867

TI NMR analysis of a conformational transition in an acyclic peptide. Model system for studying helix unfolding

AU Raghothama, S.; Chaddha, M.; Balaram, P.

CS Molecular Biophysics Unit, Indian Institute of Science, Bangalore, 560 012, India

SO J. Phys. Chem. (1996), 100(50), 19666-19671

CODEN: JPCHAX; ISSN: 0022-3654

DT Journal

LA English

CC 6-3 (General Biochemistry)

Section cross-reference(s): 34

- AB The stabilization of helical structures in short apolar peptides is readily achieved by introduction of .alpha.,.alpha.-dialkylamino acids. The use of stereochem. constrained residues in conjunction with conformationally flexible segments permits the design of peptides that are poised to undergo structural transitions. The octapeptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe (Ac8c = 1-aminocyclooctane-1-carboxylic acid) incorporates residues with contradictory conformational tendencies. NMR anal. in CDCl₃, using nuclear Overhauser effects and delineation of hydrogen-bonded NH groups establishes a 310-helical conformation. In a polar strongly solvating medium, like DMSO, the helix unfolds. Studies in CDCl₃/DMSO mixts. provide clear evidence for a solvent dependent conformational transition. Amide NH chem. shifts and temp. coeffs. at varying solvent compn. allow a detailed structural anal. of the unfolding process. The intrinsic fragility of the octapeptide helix provides an opportunity to examine invasion of the helix backbone by

water mols. Studies in DMSO soln. contg. low concns. of water establish that preferential water peptide interactions may indeed be present.

ST helix unfolding NMR model acyclic octapeptide

IT Hydrogen bond
Nuclear magnetic resonance
Overhauser effect
Simulation and Modeling, biological
(NMR anal. of conformational transition in acyclic peptide
Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)

IT Peptides, properties
RL: PRP (Properties)
(helix unfolding; NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)

IT Conformation and Conformers
(helical, NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)

IT **183667-57-4**
RL: PRP (Properties)
(Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe; NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)

IT 67-68-5, DMSO, biological studies 865-49-6
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)

L66 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:288176 HCAPLUS

DN 124:336177

TI Effect of N.alpha.-Acyl Chain Length on the Membrane-Modifying Properties of Synthetic Analogs of the Lipopeptaibol Trichogin GA IV

AU Toniolo, C.; Crisma, M.; Formaggio, F.; Peggion, C.; Monaco, V.; Goulard, C.; Rebuffat, S.; Bodo, B.

CS Department of Organic Chemistry, University of Padova, Padua, 35131, Italy

SO J. Am. Chem. Soc. (1996), 118(21), 4952-4958
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

CC 6-6 (General Biochemistry)
Section cross-reference(s): 34

AB Trichogin GA IV, an 11-residue lipopeptaibol blocked at the N-terminus by an n-octanoyl group and at the C-terminus by a 1,2-amino alc. (L-leucinol), extd. from the fungus *Trichoderma longibrachiatum*, exhibits remarkable membrane-modifying properties. We have synthesized trichogin GA IV and several [L-Leu-OMe₁₁] analogs carrying at the N-terminus an acyl chain of variable length (C2-C8, C10, C12, C14, C16, C18). A succinylated head-to-head dimer was also prepd. A conformational anal., carried out by FTIR absorption, CD, and NMR, showed that the right-handed helical structure of the natural lipopeptaibol is essentially preserved in all its analogs. Permeability measurements revealed that at least six carbon atoms in the N.alpha.-blocking fatty acyl moiety are required for the onset of significant membrane-modifying properties. Also the head-to-head dimer is remarkably active. Possible models for the mechanism of membrane permeability of trichogin GA IV are discussed.

ST lipopeptaibol trichogin GA IV membrane permeability; lipopeptide trichogin analog prepn membrane permeability

IT Antibiotics
Conformation and Conformers
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)

- IT Lipopeptides
 RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
- IT Molecular structure-biological activity relationship
 (membrane permeability-affecting, synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
- IT Biological transport
 (permeation, synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
- IT 138531-93-8P, Trichogin GA IV 173739-68-9P 176664-85-0P 176664-86-1P 176664-87-2P 176664-88-3P 176664-89-4P 176664-90-7P 176664-91-8P 176664-92-9P 176664-93-0P 176664-94-1P 176664-95-2P 176664-96-3P
 RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
- IT 99176-53-1 106897-28-3 106897-29-4 125615-20-5 141745-54-2 176664-97-4 176664-98-5 176664-99-6 176665-00-2 176665-01-3 176665-02-4 176665-03-5 176665-04-6 176665-05-7 176665-06-8 176665-07-9 176665-08-0 176665-09-1 176665-10-4 176665-11-5
 RL: PRP (Properties); RCT (Reactant)
 (synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
- IT 543-20-4, Butanedioyl dichloride 1212-53-9 2018-66-8 2666-93-5 3160-59-6 4818-03-5 15030-72-5 15030-74-7 54793-59-8 176664-71-4 176664-72-5 176665-12-6
 RL: RCT (Reactant)
 (synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
- IT 119768-28-4P 156916-67-5P 164575-77-3P 173739-67-8P 173739-69-0P 176664-73-6P 176664-74-7P 176664-75-8P 176664-76-9P 176664-77-0P 176664-78-1P 176664-79-2P 176664-80-5P **176664-81-6P** 176664-82-7P 176664-83-8P 176664-84-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)

L66 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1993:443723 HCAPLUS

DN 119:43723

TI Orientation change of glycopeptide in lipid bilayer membrane induced by lectin binding

AU Otoda, Kazuya; Kimura, Shunsaku; Imanishi, Yukio

CS Dep. Polym. Chem., Kyoto Univ., Yoshida Honmachi, Sakyo-ku, Kyoto, Japan

SO Biochim. Biophys. Acta (1993), 1145(1), 33-41

CODEN: BBACAQ; ISSN: 0006-3002

DT Journal

LA English

CC 6-6 (General Biochemistry)

AB A lectin-induced orientation change of a helical glycopeptide in lipid bilayer membranes was studied. Glycopeptides composed of hydrophobic nona-(G8) and pentapeptide (G4) with a fluorescent probe at the N-terminal and a lactose unit at the C-terminal were synthesized. The glycopeptides were incorporated into lipid bilayer membranes (BLM) with the lactose unit exposed to the aq. phase and the peptide chain buried in the membrane. G8

- takes a partially helical structure in the membrane, while G4 an irregular structure. Upon binding of lectin to G8 held in the membrane of dipalmitoylphosphatidylcholine (DPPC) liposome, enhancement of fluorescence intensity of the N-terminal anthryl group, redn. of fluorescence quenching of the anthryl group with acrylamide, and increase of CF-leakage from the DPPC liposome were obsd. G8', which lacks the O-anthrilmethylserine residue from G8, formed a voltage-dependent ion channel in BLM expts. The frequency of single current fluctuations induced by G8' incorporation increased with addn. of lectin. These results indicate that the peptide segment of G8 prefers taking a more perpendicular orientation to the membrane upon assocn. with lectin.
- ST glycopeptide helix phosphatidylcholine bilayer orientation lectin;
agglutinin RCA60 glycopeptide membrane orientation; ion channel
glycopeptide bilayer membrane
- IT Agglutinins and Lectins
RL: BIOL (Biological study)
(RCA60, helical glycopeptide orientation in phosphatidylcholine bilayer membrane response to)
- IT Phosphatidylcholines, biological studies
RL: BIOL (Biological study)
(bilayer membrane, glycopeptide orientation in, lectin effect on)
- IT Ion channel
(formation of voltage-dependent, by glycopeptide and hydrophobic helical peptide in phospholipid planar bilayer)
- IT Molecular orientation
(of helical glycopeptide, in phosphatidylcholine bilayer membrane, lectin effect on)
- IT Glycopeptides
RL: PRP (Properties)
(orientation of, in phosphatidylcholine bilayer membrane, lectin effect on)
- IT Membrane, biological
(bilayer, phosphatidylcholine, glycopeptide orientation in, lectin effect on)
- IT Electric activity
(current-potential relationship, of glycopeptide and hydrophobic helical peptide ion channel in phospholipid planar bilayer)
- IT Conformation and Conformers
(.alpha.-helical, of glycononapeptide in phosphatidylcholine bilayer membrane)
- IT 2644-64-6, Dipalmitoylphosphatidylcholine 13699-48-4,
Dimyristoylphosphatidylcholine
RL: BIOL (Biological study)
(bilayer membrane, glycopeptide orientation in, lectin effect on)
- IT 148505-61-7P 148505-62-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation and orientation in phosphatidylcholine bilayer membrane of, lectin effect on)
- IT 74426-35-0P 148505-59-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling with peptide derivs. of)
- IT **148505-60-6P** 148526-29-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling with serine derivs. of)
- IT 148526-30-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenation of)
- IT 148505-63-9P 148505-64-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydroxylation of)
- IT 136198-08-8P 148505-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ion channel formation in phospholipid bilayer by)
- IT 5965-65-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with benzyloxycarbonylethylenediamine)

- hydrochloride of)
- IT 148526-31-2P 148526-32-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with lactose derivs. of)
- IT 3262-72-4
RL: RCT (Reactant)
(reaction of, with chloromethylantracene and sodium hydride)
- IT 18807-71-1, N-Benzyloxycarbonylethylenediamine hydrochloride
RL: RCT (Reactant)
(reaction of, with lactonolactone)
- IT 7646-69-7, Sodium hydride
RL: RCT (Reactant)
(reaction of, with serine derivs. and chloromethylantracene)
- IT 24463-19-2, 9-Chloromethylantracene
RL: RCT (Reactant)
(reaction of, with serine derivs. and sodium hydride)
- L66 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1992:572078 HCAPLUS
DN 117:172078
TI Changes in conformation and antimicrobial properties caused by replacement
of D-amino acids with .alpha.-aminoisobutyric acid in the gramicidin
backbone: synthesis and circular dichroic studies
AU Jelokhani-Niaraki, Masood; Yoshioka, Katsumi; Takahashi, Hiroki; Kato,
Fumio; Kondo, Michio
CS Fac. Sci. Eng., Saga Univ., Saga, 840, Japan
SO J. Chem. Soc., Perkin Trans. 2 (1992), (7), 1187-93
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 10, 22
- AB In an attempt to mimic the stable helical structures of proteins with
possible pore-forming ability in membranes, the linear gramicidin backbone
has been changed by inserting achiral .alpha.-aminoisobutyric acids (Aib)
in place of all the alternatively sequenced D-amino acids. The
conformation and biol. activity of the synthetic gramicidin A and B
analogs have been studied. CD measurements have been used to det. the
conformation in soln. The original conformation of gramicidin clearly
changes and its antimicrobial activity is reduced in Aib analogs.
Although .alpha.-helical motifs can be clearly distinguished in analogs,
the CD spectra show inherent complexities. The possibility of
superposition of different conformations is considered. The potential
pore-forming ability of analogs is briefly discussed.
- ST aminoisobutyric acid analog gramicidin conformation; structure activity
bactericide gramicidin analog
- IT Conformation and Conformers
(of .alpha.-aminoisobutyric acid-contg. gramicidin analogs)
- IT Bactericides, Disinfectants, and Antiseptics
(.alpha.-aminoisobutyric acid-contg. gramicidin analogs)
- IT Molecular structure-biological activity relationship
(bactericidal, of .alpha.-aminoisobutyric acid-contg. gramicidin
analog)
- IT 1405-97-6P, Gramicidin
RL: SPN (Synthetic preparation); PREP (Preparation)
(aminoisobutyric acid-contg. analogs, prepn., conformation, and
bactericidal activity of)
- IT 1161-13-3, N-Benzyloxycarbonylphenylalanine 2002-24-6, 2-Aminoethanol
hydrochloride 5680-79-5, Glycine methyl ester hydrochloride 7432-21-5
13734-41-3 15028-41-8, .alpha.-Aminoisobutyric acid methyl ester
hydrochloride 15761-38-3, N-tert-Butoxycarbonylalanine
RL: RCT (Reactant)
(peptide coupling reactions of, in prepn. of gramicidin analogs)
- IT 143868-49-9P 143868-66-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and catalytic hydrogenolysis)

IT 2637-44-7P 143868-54-6P 143868-61-5P 143868-68-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and catalytic hydrogenolysis of)

IT 66449-52-3P 143868-56-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of, with hydrogen chloride)

IT 143868-62-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of, with trifluoroacetic acid)

IT **143868-51-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and formylation of)

IT 143868-48-8P 143868-65-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, in prepn. of gramicidin analog)

IT 143868-47-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, in prepn. of gramicidin analogs)

IT 143868-53-5P 143868-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide deriv. in prepn. of
gramicidin analog)

IT 1685-28-5P 85918-88-3P 89045-43-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide deriv. in prepn. of
gramicidin analogs)

IT 143868-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation).
(prepn. and peptide coupling of, with dipeptide derivs. in prepn. of
gramicidin analogs)

IT 45233-75-8P 72095-04-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide ester in prepn. of
gramicidin analogs)

IT 143868-59-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tetrapeptide deriv. in prepn. of
gramicidin analogs)

IT 143868-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tetrapeptide ester in prepn. of
gramicidin analogs)

IT 109772-33-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tetrapeptide in prepn. of
gramicidin analog)

IT 143868-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling reactions of, in prepn. of gramicidin
analog)

IT 51803-69-1P 98714-71-7P 143868-50-2P 143868-55-7P 143868-63-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

IT 143868-46-6P 143868-64-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and bactericidal activity of)

IT 72086-77-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., deblocking, or sapon. of)

L66 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1988:590816 HCAPLUS

DN 109:190816

TI Synthesis of linear undecapeptide precursors of cyclosporin analogs

AU Galpin, I. J.; Mohammed, A. K. A.; Patel, A.

CS Robert Robinson Lab., Univ. Liverpool, Liverpool, L69 3BX, UK

SO Tetrahedron (1988), 44(6), 1773-82
CODEN: TETRAB; ISSN: 0040-4020

DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
OS CASREACT 109:190816

AB Eleven protected undecapeptide precursors of cyclosporin analogs were
prepd. by stepwise elongation of PhCH₂O₂C-(4-11)-OCMe₃ using the
diphenylphosphinic mixed anhydride method. Yields were in the 60-90%
range and optically pure peptides were obtained. A no. of fragment
condensations approaches were studied; the diphenylphosphinic anhydride
fragment coupling gave only a 39% yield.

ST cyclosporin analog undecapeptide precursor

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(undeca-, prepn. of, as precursors of cyclosporin analogs)

IT 28920-43-6
RL: RCT (Reactant)
(acylation by, of threonine deriv.)

IT 82911-69-1
RL: RCT (Reactant)
(fluorenylmethoxycarbonylation by, of diaminobutyric acid)

IT 1883-09-6 42417-72-1
RL: RCT (Reactant)
(fluorenylmethoxycarbonylation of)

IT 16966-09-9 42417-73-2 42918-86-5
RL: RCT (Reactant)
(peptide coupling of)

IT 39608-31-6
RL: RCT (Reactant)
(peptide coupling of with octapeptide deriv.)

IT 21691-44-1, N-Benzylloxycarbonyl-L-norvaline 39608-30-5,
N-Benzylloxycarbonyl-L-norleucine
RL: RCT (Reactant)
(peptide coupling of, with nonapeptide deriv.)

IT 117106-30-6
RL: RCT (Reactant)
(peptide coupling of, with octapeptide deriv.)

IT 117106-24-8
RL: RCT (Reactant)
(peptide coupling of, with sarcosine deriv.)

IT 117106-31-7
RL: RCT (Reactant)
(peptide coupling of, with tripeptide deriv.)

IT 116236-40-9P 116823-65-5P 117106-17-9P 117106-18-0P 117129-76-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenolysis of)

IT 85201-91-8P 117106-19-1P 117106-20-4P 117106-21-5P 117106-25-9P
117106-26-0P 117106-27-1P 117106-28-2P 117106-29-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of)

IT 117106-23-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

IT 117106-22-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tert-butoxycarbonylation of)

IT 116236-39-6P 116236-41-0P 116236-42-1P 116236-43-2P 116236-44-3P
116236-45-4P 116236-46-5P 116236-47-6P 116236-48-7P 116236-49-8P
116236-50-1P 116236-51-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 79217-60-ODP, Cyclosporin, analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of linear undecapeptide precursors of)

IT 1676-75-1

RL: RCT (Reactant)
(N-methylation of)

IT 115-11-7, Isobutylene, reactions
RL: RCT (Reactant)
(O-tert-butylation by, of hydroxyproline deriv.)

IT 112203-99-3
RL: RCT (Reactant)
(O-tert-butylation of, with isobutylene)

L66 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1986:104617 HCAPLUS
DN 104:104617
TI Vibrational circular dichroism of polypeptides, V. A study of
310-helical-octapeptides
AU Yasui, Sritana C.; Keiderling, Timothy A.; Bonora, Gian Maria; Toniolo,
Claudio
CS Dep. Chem., Univ. Illinois, Chicago, IL, 60680, USA
SO Biopolymers (1986), 25(1), 79-89
CODEN: BIPMAA; ISSN: 0006-3525
DT Journal
LA English
CC 6-3 (General Biochemistry)

AB Vibrational CD spectra were measured in the 3600-1250 cm⁻¹ region of 2
monodisperse, protected octapeptides which form right-handed 310-helices
in CDCl₃ soln. The spectra are similar in sign pattern to those obtained
for right-handed α -helices in soln. but are smaller in magnitude
and, addnl., provide evidence of some line-shape differences. The
delineation of this type of ordered conformation was accomplished by means
of ¹H NMR. Such a soln. structure is consistent with the x-ray crystal
structure of 1 of these mols.

ST vibrational CD peptide conformation; helix 3 10 protein vibrational CD
IT Peptides, properties
Proteins
RL: PRP (Properties)
(conformation of, 310-helical, vibrational CD in relation to)

IT Infrared spectra
Nuclear magnetic resonance
(of peptides, vibrational CD in relation to)

IT Conformation and Conformers
(310-helical, of proteins, vibrational CD in relation to)

IT Crystal structure-property relationship
(conformation, of peptides)

IT 72485-35-9
RL: RCT (Reactant)
(deprotection of)

IT 100817-47-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and vibrational CD spectra of, 310-helical conformation in
relation to)

IT 90892-16-3
RL: RCT (Reactant)
(reaction of, with aminoisobutyrate polymer oxazolone)

IT 4512-43-0
RL: RCT (Reactant)
(reaction of, with leucylisobuteroaminoisobutyrate Me ester)

IT 95842-05-0 **100843-78-5**
RL: PRP (Properties)
(vibrational CD spectra of, 310-helical conformation in relation to)

L66 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1979:187312 HCAPLUS
DN 90:187312
TI Carbon-13 NMR spectroscopic studies on the conformation during stepwise
synthesis of peptides bound to solubilizing polymer supports
AU Leibfritz, D.; Mayr, W.; Oekonomopulos, R.; Jung, G.
CS Inst. Org. Chem., Univ. Frankfurt, Frankfurt, Ger.

SO Tetrahedron (1978), 34(13), 2045-50
CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

CC 34-3 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22, 35

AB The ¹³C (¹³C-¹H) triple resonance technique was applied to constitutional and conformational studies of polypeptides bound to mono- and bifunctional solubilizing polyoxyethylene supports. High resoln. showed distinct differences between random coil and .alpha.-helical conformations. This method is valuable for the control of the growing peptide during stepwise synthesis on sol. polymeric supports. Examples of partial sequences of alamethicin and sequential analogs demonstrate the applicability to peptide polyoxyethylene esters with mean mol. wts. of 2000-10,000.

ST polyoxyethylene bound peptide conformation NMR; alamethicin conformation carbon NMR; Merrifield peptide prepn carbon NMR

IT Peptides, properties
RL: PRP (Properties)
(conformation of polymer-bound, carbon-13 NMR detn. of)

IT Merrifield synthesis
(of peptides, conformational control in, carbon-13 NMR in relation to)

IT Conformation and Conformers
(of polyoxyethylene-bound peptides, carbon-13 NMR detn. of)

IT Nuclear magnetic resonance
(carbon-13, in polyoxyethylene-bound peptides)

IT 13726-85-7D, polymer-bound 13734-41-3D, polymer-bound 32991-17-6D,
polymer-bound 70134-38-2D, polymer-bound 70134-39-3D, polymer-bound
70134-40-6D, polymer-bound 70134-41-7D, polymer-bound 70134-42-8D,
polymer-bound **70134-43-9D**, polymer-bound 70134-44-0D,
polymer-bound
RL: PRP (Properties)
(conformation of, carbon-13 NMR detn. of)